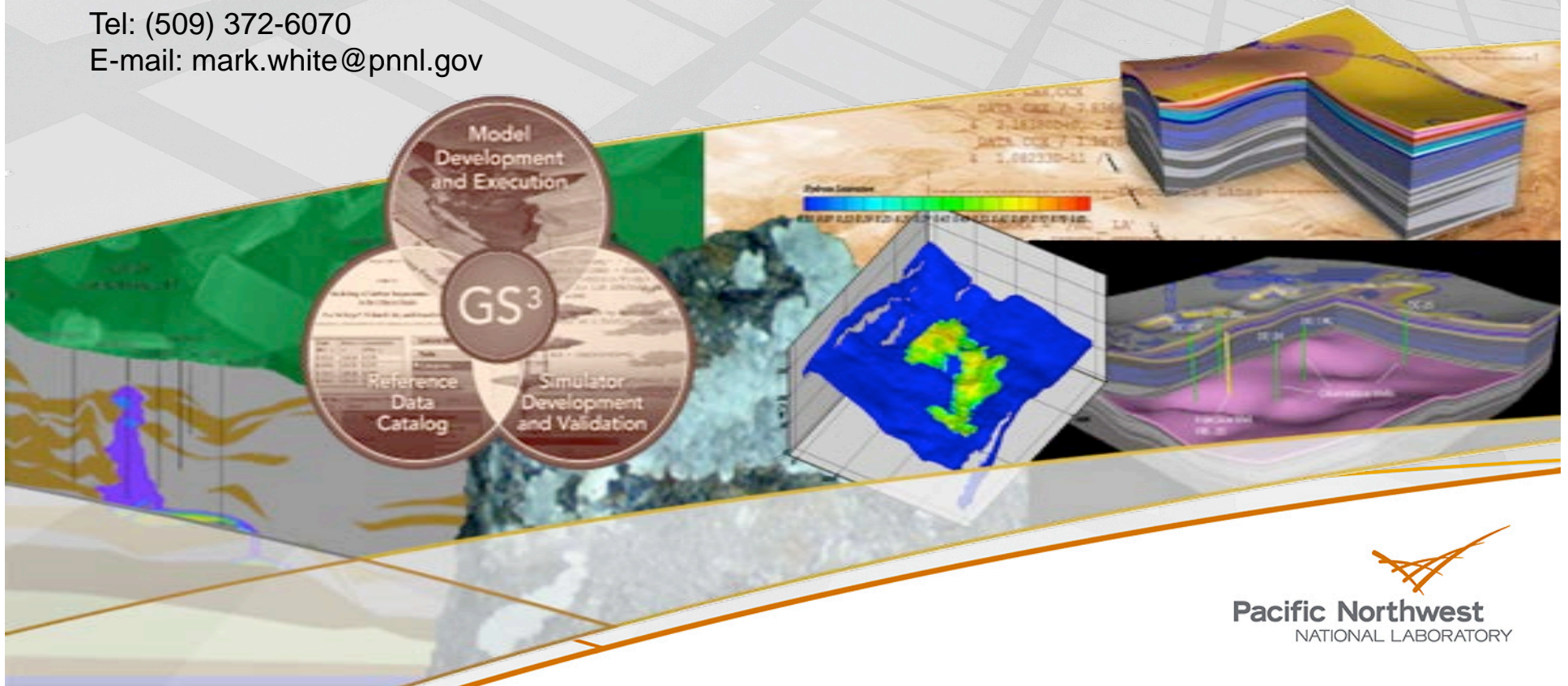


Reservoir Modeling Working Group Meeting Information
2012 Geothermal Technologies Program Peer Review
Westminster, Colorado, May 10, 2012

Discussion on a Code Comparison Effort for the Geothermal Technologies Program

Mark White, Ph.D., P.E.
Senior Research Engineer
Hydrology Group
PNNL
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E-mail: mark.white@pnnl.gov



Colleague



Dr. Timothy D. (Tim) Scheibe was selected as the 2010 Henry Darcy Distinguished Lecturer in Ground Water Science. Scheibe, a staff scientist at Pacific Northwest National Laboratory, was invited by the National Ground Water Research and Educational Foundation to spend next year lecturing at colleges and universities to educate and create interest in groundwater science and technology.

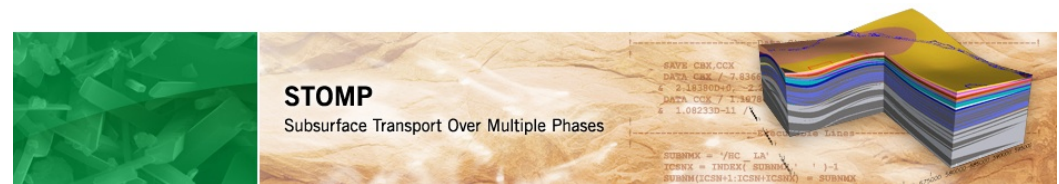
- Lectures and faculty/student meetings
- Roughly 40 host institutions across the United States and internationally
- Beyond the Black Box: Integrating Advanced Characterization of Microbial Processes with Subsurface Reactive Transport Models
- Quantifying Flow and Reactive Transport in the Heterogeneous Subsurface Environment: From Pores to Porous Media and Facies to Aquifers

E-mail: tim.scheibe@pnnl.gov



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Topics



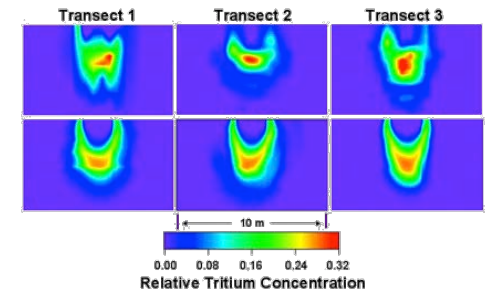
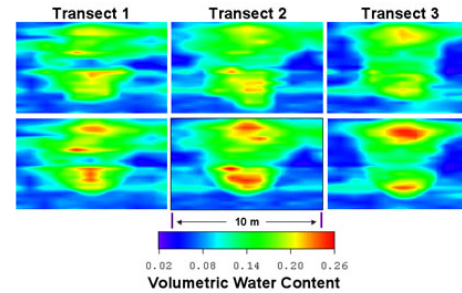
- PNNL's Participation in Code Comparisons
- Code Comparison Observations
- Preliminaries for a Geothermal Reservoir Code Comparison
- VELO: Knowledge Management Framework for Modeling and Simulation
- STOMP: PNNL's Subsurface Flow and Transport Simulator



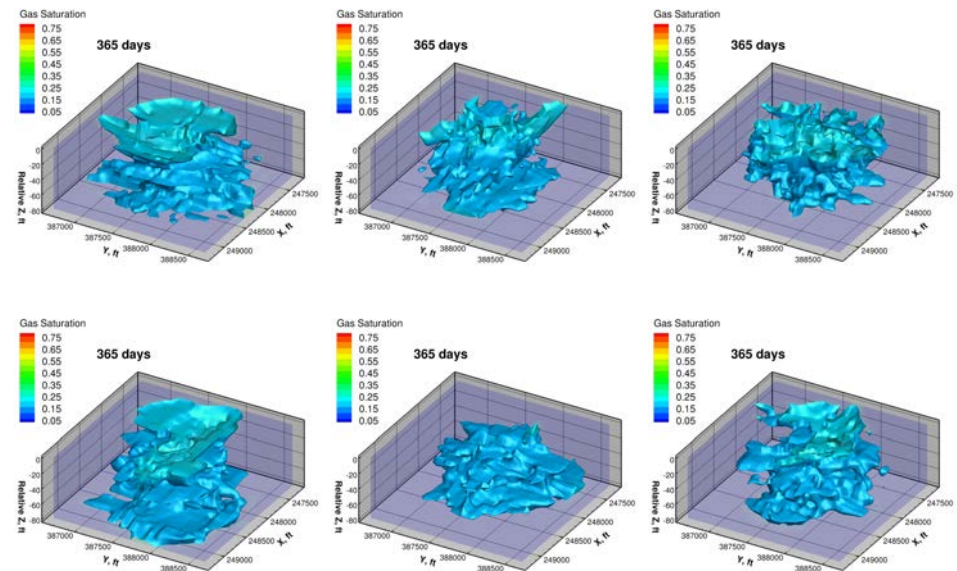
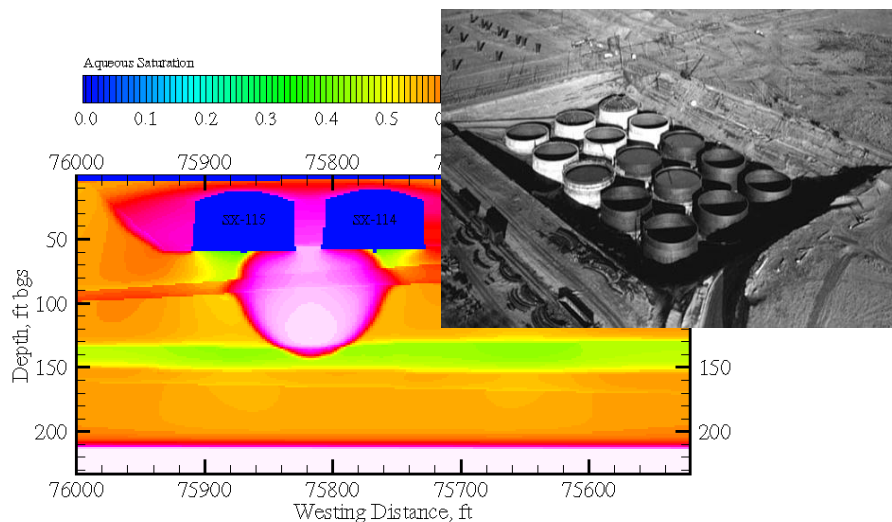
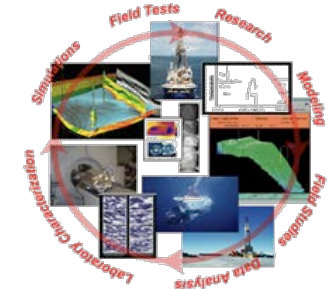
Code Comparisons



- Las Cruces Trench (1993)
- Yucca Mountain (1994)
- Hanford Site (1999)
- GeoSeq (2002)
- International Hydrate Code Comparison (2007)
- Sim-SEQ (2011)



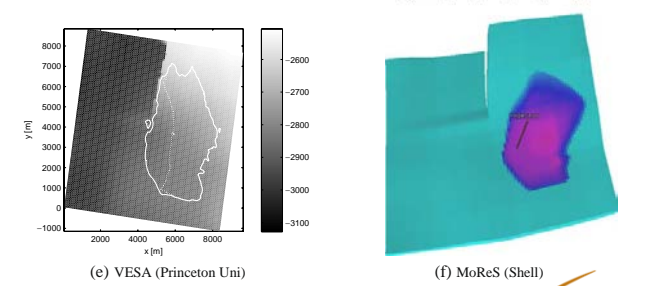
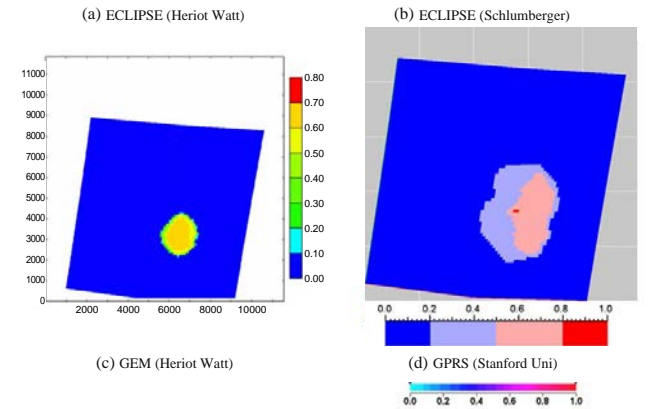
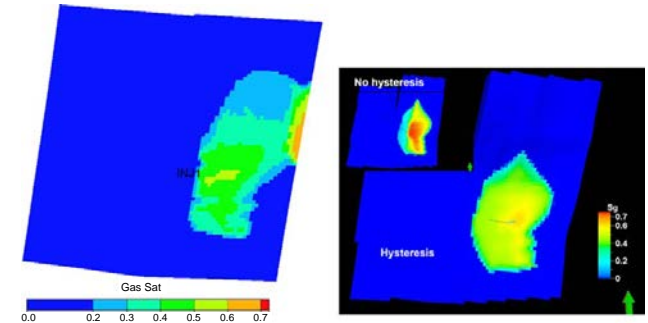
GEO-SEQ



Observations



- Blind comparisons
 - Detract from open scientific exchanges
 - Emphasis on coding errors
 - Daunting for new modeling groups
 - Reminiscent of looking up posted grades
- Problem Complexity
 - Core benchmarking problems are essential
 - Early comparisons bond the modeling groups
 - Legacy of increasing problem complexity invites future teams
 - Complex problems will generate differences in results



Observations



- Problem Definitions

- Collective agreement on problem types increases participation
- Single author problem descriptions were generally more complete and more comprehensible
- Collective review of the problem descriptions diminishes differences in code capabilities
- Data collection details need to be included for field data comparisons

- Participants

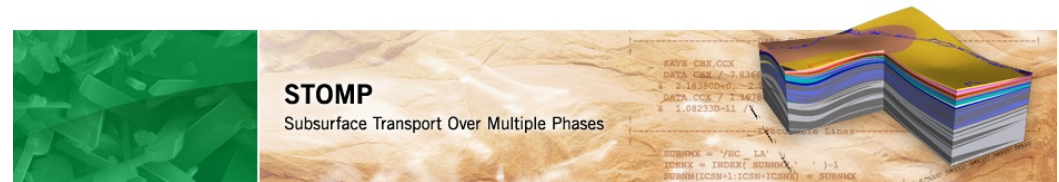
- Diversity is an asset.
- Kickoff workshop promotes collaborative discourse in future conference calls
- Rotating conference call times encourages international participation



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Observations



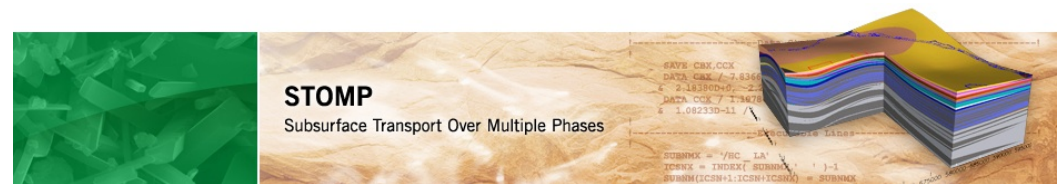
- Simulators

- Research codes have the greatest flexibility for change.
- Industrial codes need financial motivation to change.
- Commercial codes are generally the least flexible and least open with respect to details and numerical schemes.
- Flexible commercial codes allow for diverse modeling approaches.
- Academic licenses for commercial codes are considerably less than their profession equivalents

- Technology Transfer

- Public website invites interest and new modeling teams
- Combined joint and individual publications are effective
- Special edition publications motivate modeling teams

Perspective

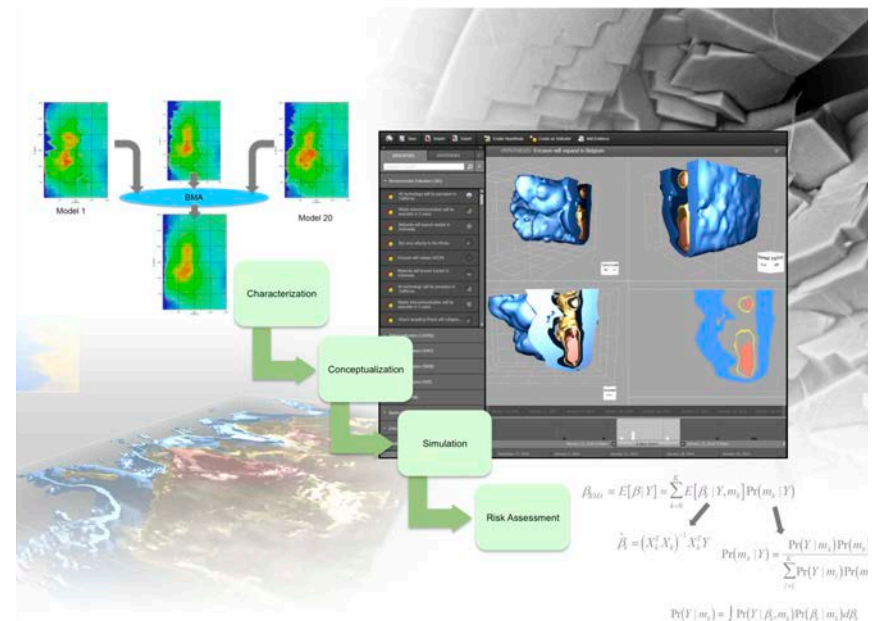


- International community with governmental agency, national laboratory, independent research, industrial, and academic representation.
- Kickoff workshop.
- Repository of progressively more complex EGS problems.
- Simple problems isolate thermodynamics, hydrodynamics, rock mechanics, and geochemistry.
- Analytical, code inter-comparison, laboratory data, field data.
- Collaborative but secure computational framework.
- Public access to problems and simulation results.
- Publication of findings.

Preliminaries



- Soliciting national and international participation
- Developing a set of protocols and comparison procedures
- Planning a kick-off workshop
- Creating an instance of VELO for the Geothermal Technologies Program

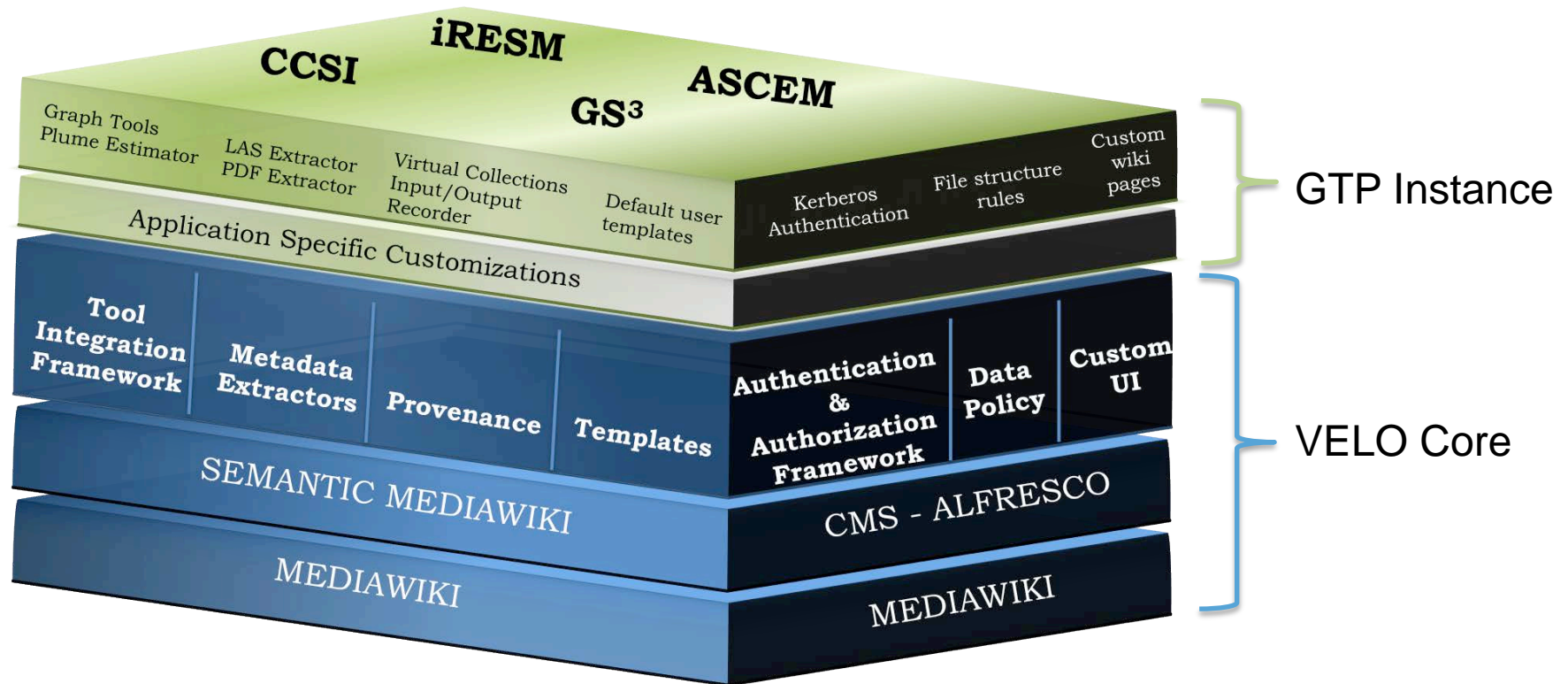




A flexible, foundational, collaborative technology that can be used in modeling and simulation projects to

- capture, organize, query, and share experimental and observational data, along with the scientific processes and reasoning that are used to develop computational models
- provide versioning of model inputs for specific projects and provenance for simulation results
- enable simulations to be launched on remote computational platforms
- support both tight and loose integration of third-party tools to facilitate various modeling activities, such as model development and visualization

VELO Architecture



- **MEDIAWIKI:** provides a collaborative and extensible user environment
- **ALFRESCO:** manages complex, large data sets used in scientific modeling
- **SEMANTIC MEDIAWIKI:** provides semantic markup and search capabilities

VELO Page



1. File Manager
2. Scratchpad
3. Tool Access and Navigation
4. Content Area
5. Wiki Functions

The screenshot displays the VELO web interface. At the top, there's a navigation bar with 'Home', 'Browse', 'Tools', 'Misc. Tools', 'Account Links', and 'Help'. A search bar is on the right. Below the navigation bar, there's a 'Scratchpad' section with a list of PDF files: 'Person_2010.pdf' and 'Revil_2000.pdf'. To the left of the main content area is a 'File Manager' section with a grid icon. The main content area shows a PDF document titled 'WFS:/refdata/Mt Simon refs/Leetaru 2009.pdf'. The document content includes a table of facts about the PDF, such as 'Agencies: Department of Energy/DOE;2', 'Analysis methods: stochastic(approach);1', 'Data Identifiers: Core (8), Wells (4), and Log(s)/ged/ging (1)', 'Depositional Environment: Basin(s) (25), and Margin(s) (1)', 'Geologic Period: Cambrian (3), Precambrian (2), and Ordovician (1)', 'Qualitative Rock Or Sediment: Arkosic (4)', 'Description: Sandstone (11), and Shale (3)', 'Rock Name: Sandstone (11), and Shale (3)', and 'Rock Property: Thick(ness) (21), Permeabilit(y/ies) (6), Porosit(y/ies) (5), Compressibility (5), and Depth(s) (1)'. Below the table is a 'Back to Parent' link and a PDF icon. At the bottom, there's a 'PDF First Page Preview' section with a file size of 2.39 MB and a MIME type of application/pdf. The interface is annotated with red numbers 1 through 5, corresponding to the list items on the left.

VELO Instances



SimSEQ

Home | Browse | Tools | Misc. Tools | Account Links | Help

UserLogin > /projects/Sim-SEQ/Imperial London/Day33 3 Jan 2010.txt > /projects/Sim-SEQ/Imperial London > /users/Admin >

Tool Input
ScratchPad | FileManager

Scratchpad

File Manager

WFS:/users/Admin/satellite--image.jpg

Back to Parent

Firefox

CAT/Natural--Communities--Projects--Hypersaline--Mat

http://microbes.pnl.gov/wiki/index.php/CAT/Natural--Communities--Projects/Hypersaline--Mat

Currently Logged in as: Lmccue | Logout

U.S. DEPARTMENT OF ENERGY | Microbes FSFA

FSFA Wiki Home | About | Browse Data | Forum | Toolbox

CAT Browser

- Omic
- Admin
- Collaborations
- Geochemistry
- Hot-Lake-Site
- Hot-Lake-Team
- Microbiology
- Modeling
- Pigmentation
- Proposals--Papers--Posters--Presentations
- Protocols
- Sampling

cat Edit History Watch

CAT/Natural--Communities--Projects/Hypersaline--Mat

Date Created: Fri Aug 05 17:04:21 PDT 2011

Created By: admin

Last Modified:

Project: Hypersaline--Mat

Project Title: Hypersaline--Mat

Contents [show]

Summary [edit]

Hot Lake/Hypersaline Mat Forum

Hot Lake is a meromictic, hypersaline lake that occupies a glacial endorheic basin in north-central Washington. Once mined for its epsomite, Hot Lake is notable in that it is a system high in magnesium sulfate due to weathering of mafic rocks; most hypersaline ecosystems studied to date are predominantly sodium chloride. Epsomitic hypersaline lakes are common features of the inter-range semi-arid plateau between the Rocky Mountains and the Coast and Cascade Ranges. Microbial mats have been reported to widely colonize these

integrated Regional Earth System Model (iRESM) Initiative

Home | Data | Models | Tools | Coupling | Evaluation | Demonstration

UserLogin > iRESM Home >

Tool Input
ScratchPad | FileManager

Scratchpad

File Manager

WFS:/users/Admin

My Recent Changes

Recent Changes by others

My Favorites

Help Page

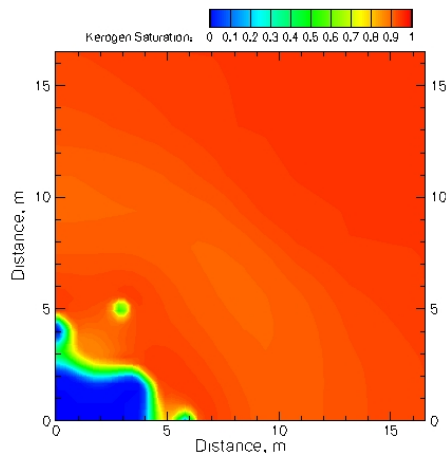
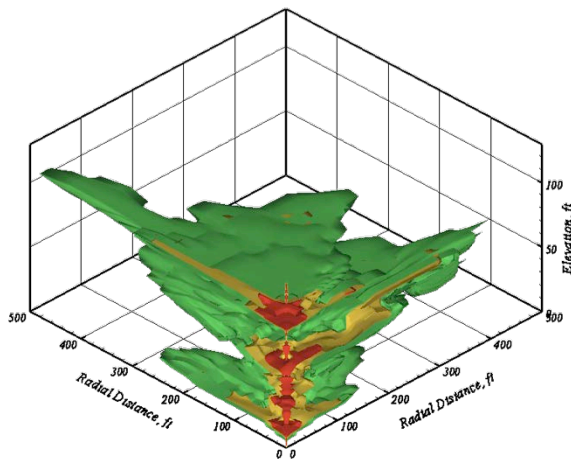
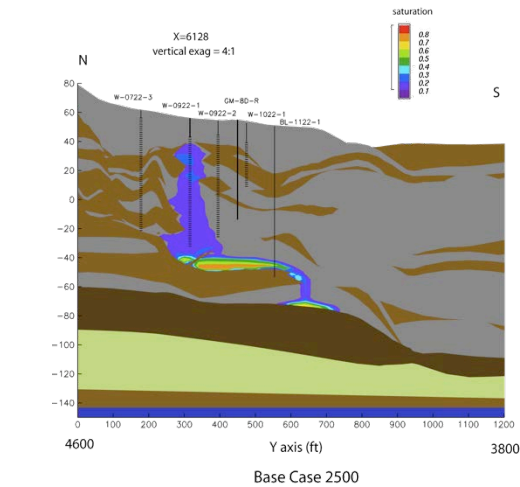
My MWM Home

STOMP at a Glance



Subsurface Transport Over Multiple Phases (STOMP) is a numerical simulator, developed at PNNL, for modeling multifluid flow and reactive transport through geologic media.

- STOMP - sequential implementation (Fortran)
- eSTOMP - scalable implementation (Fortran/Global Arrays/MPI)
- Phases - aqueous, gas, nonaqueous phase liquid, ice, hydrate, solid
- Components - water, air, oil, salt, CO₂, CH₄, noncondensable gases, heavy oils, light oils, dilute solutes, reactive species (ECKEChem)
- Thermal Environments - isothermal, nonisothermal
- Saturation Functions - nonhysteretic, entrapment, residual
- Gridding - structured (Cartesian, cylindrical, boundary fitted)
- Numerical Solvers - banded, conjugate gradient (SPLIB, Indiana University), parallel (PETSc, Argonne National Lab)
- Website - <http://stomp.pnl.gov>



Environmental Stewardship

U.S. Department of Energy legacy waste from the nuclear weapons material production era:

- Radionuclide migration and remediation
- Nuclear waste tank leakage
- Vegetated surface barrier design
- Freeze-wall technology

Environmental Remediation

U.S. Department of Energy, U.S. Department of defense, and Superfund site remediation:

- Carbon tetrachloride in deep vadose zone environment
- Trichloroethylene in arid climate
- Petrol-processing waste in shallow water table environment

Geologic CO₂ Sequestration

Industrial, U.S. Department of Energy, and regional partnership projects:

- Deep sedimentary saline formations
- Deep basaltic saline formations
- Methane hydrate formations with co-production

Hydrocarbon Production

Industrial, U.S. Department of Energy, Indian Governmental and Korean Governmental projects:

- Alaska Northslope gas hydrate accumulations
- Suboceanic gas hydrate accumulations
- Piceance Basin oil shale
- Enhanced oil recovery technologies

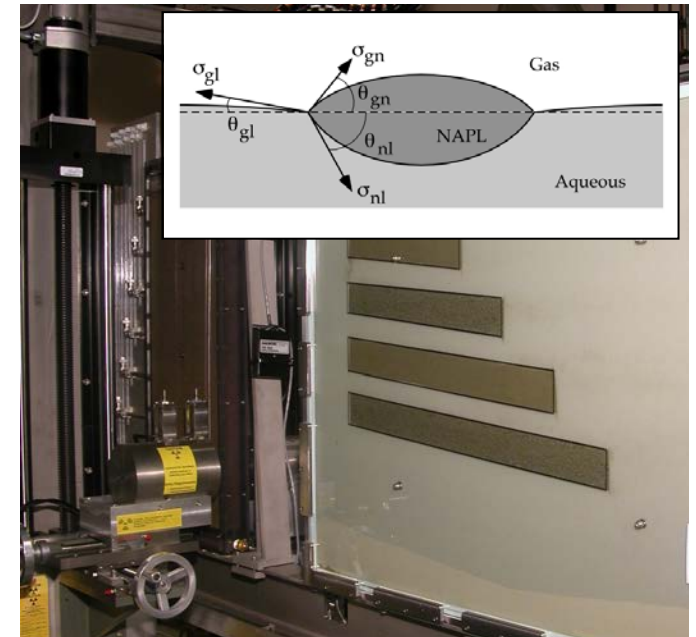
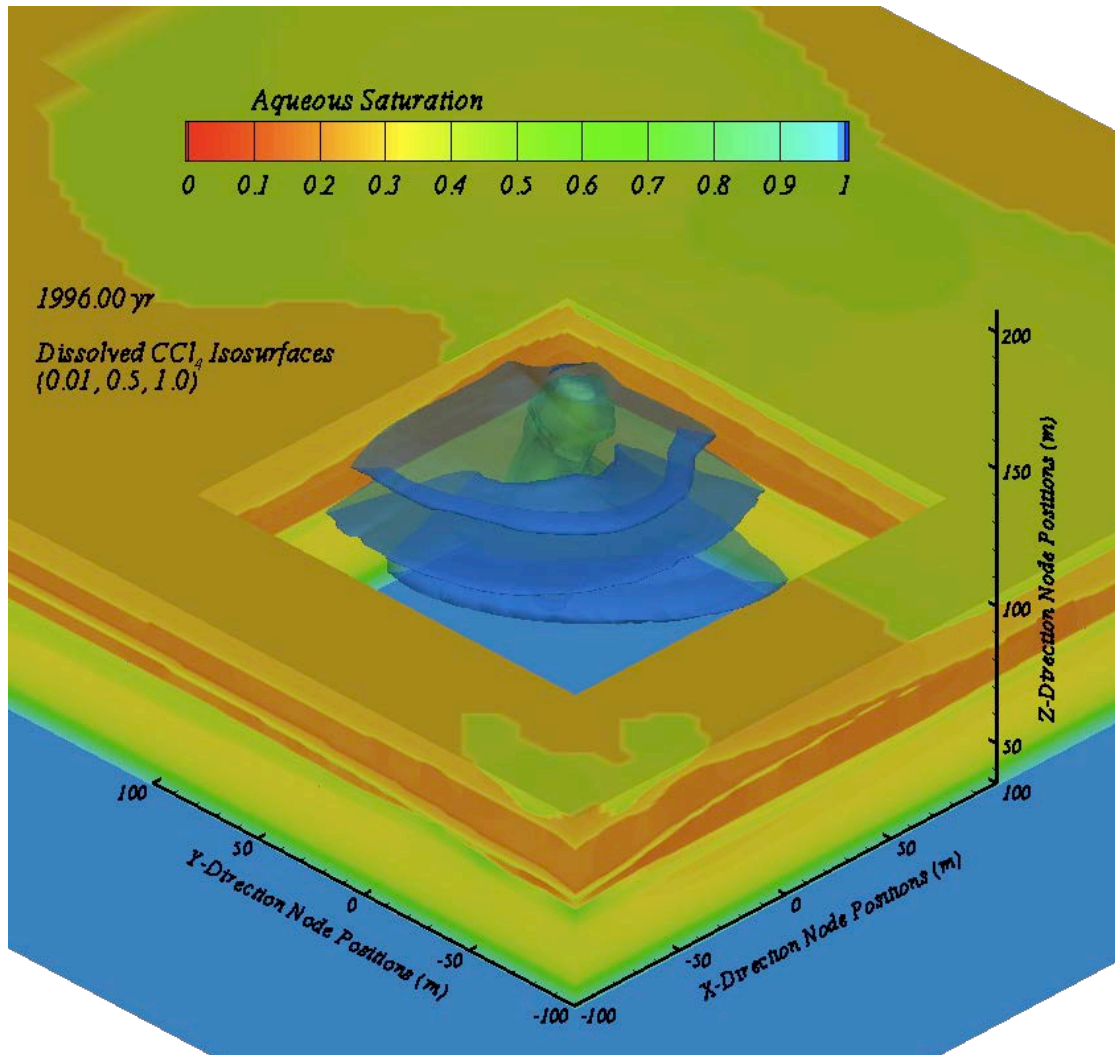


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Experimental Links



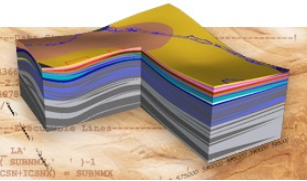
- CCl_4 Migration and Remediation
- Z-9 Crib, Hanford Site, Washington, United States



Technology Transfer



STOMP
Subsurface Transport Over Multiple Phases



KIGAM Korea Institute of Geoscience and Mineral Resources



Battelle
The Business of Innovation

Colorado State University

OSU Oregon State University



Universität Stuttgart

TU Delft

Delft University of Technology



THE UNIVERSITY OF UTAH

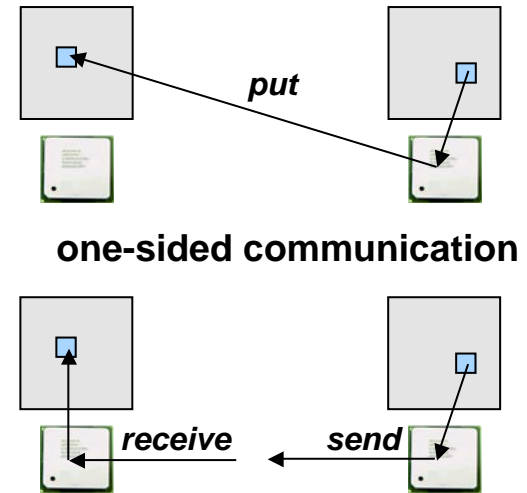
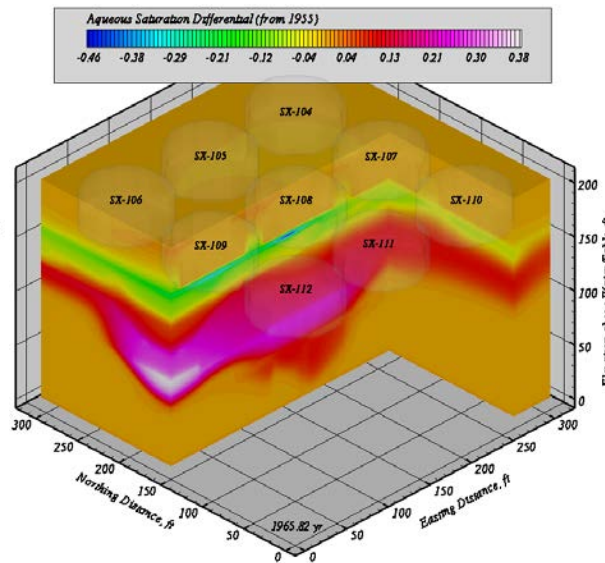
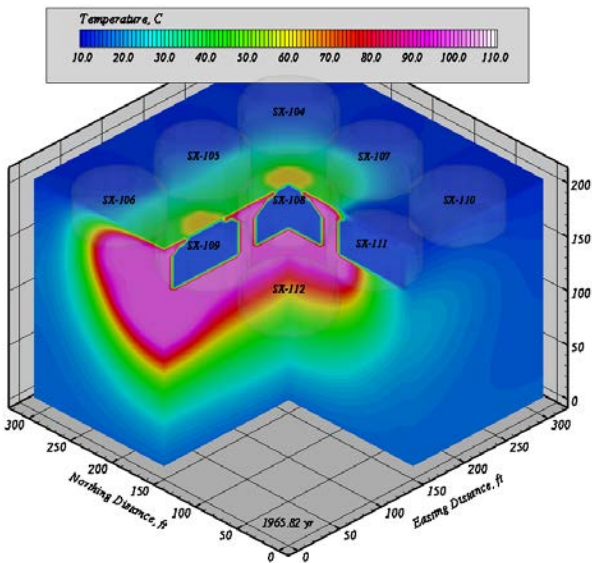
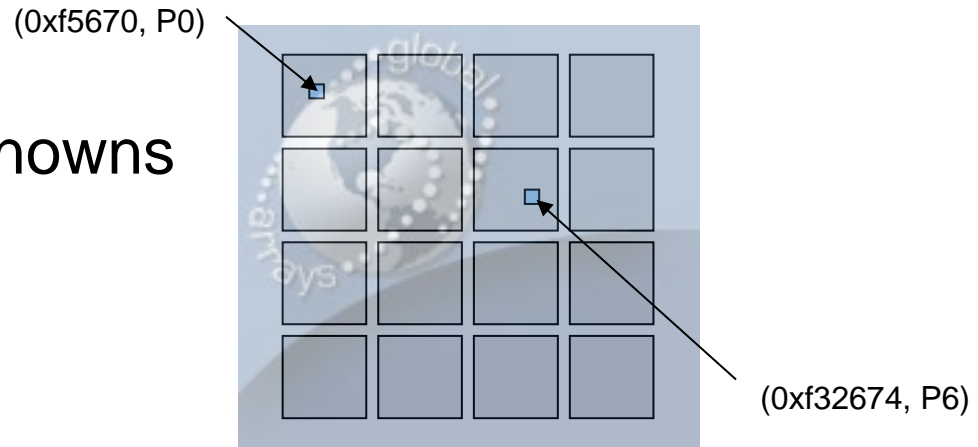
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Scalable Computing



- Global Arrays
- Implicit Solve on 1G Unknowns
- 1.4K Processors



message passing

SX Tank Farm, Hanford Site, Washington
Temperature and Aqueous Saturation: 1965.82 yr